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Understanding phonon transport in thermoelectric materials using *ab initio* approaches

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Good thermoelectric materials have low phonon thermal conductivity, k_{ph} [1]. Accurate theories to describe k_{ph} are important components in developing predictive models of thermoelectric efficiency that can help guide synthesis and measurement efforts. We have developed *ab initio* approaches to calculate k_{ph}, in which phonon modes and phonon scattering rates are computed using interatomic force constants determined from density functional theory, and a full solution of the Boltzmann transport equation for phonons is implemented [2-5]. A recent approach to calculate interatomic force constants using *ab initio* molecular dynamics [6] has yielded a good description of the thermal properties of Bi_2Te_3. But, the complexity of new promising candidate thermoelectric materials introduces computational challenges in assessing their thermal properties. An example is germanane, a germanium based hydrogen-terminated layered semiconductor [7], which we will discuss in this talk. [1] H. J. Goldsmid, Thermoelectric Refrigeration (Plenum, New York, 1964); [2] D. A. Broido et al, Appl. Phys. Lett., 91, 231922 (2007); [3] A. Kundu et al, Phys. Rev. B, 84, 125426 (2011); [4] W. Li et al, Phys. Rev. B 86, 174307 (2012); [5] Olle Hellman and I. A. Abrikosov, Phys. Rev. B 88, 144301 (2013); [6] O. Hellman and D. A. Broido, Phys. Rev. B 90, 134309 (2014); [7] E. Bianco, et al., ACS Nano 7, 4414 (2013).